

The Biomedical Ontology Applications (BOA) Framework

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Abstract. The Biomedical Ontology Applications (BOA) framework consists of a set of web applications that aim at an effective exploration of biological information and knowledge discovery using Biomedical Ontologies. This paper presents three BOA web applications: ProteInOn for semantic similarity and protein set characterization based on Gene Ontology (GO); CMPSim for semantic similarity of chemical compounds and metabolic pathways using the Chemical Entities of Biological Interest (ChEBI) ontology; and GRYFUN for the visualization, filtering and analysis of GO functional annotation profiles of a given protein family. The web tools and their documentation, including videos, are freely available from <http://xldb.di.fc.ul.pt/wiki/BOA>

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1 Introduction

The Biomedical Ontology Applications (BOA) framework integrates biomedical ontologies and databases with a number of algorithms and visualization tools, focusing on ontology-based semantic similarity. The BOA web tools, ProteInOn, CMPSim and GRYFUN, are interconnected, and currently support functional analyses that encompass chemical compounds, gene products and metabolic pathways.

2 BOA Web Tools

ProteInOn (Protein Interactions & Ontology) integrates data from the Gene Ontology (GO) [1], GOA, IntAct [2] and UniProt [3] databases. It provides eight GO-based semantic similarity measures [4,5] that can be applied to proteins or GO terms across the three GO aspects. It also supports the identification of the most meaningful functional annotations of a given set of proteins, based on the probability of annotation of each GO term, and the retrieval of interacting proteins. The integration of these features supports complex analysis such as candidate gene identification [6].

CMPSim (Chemical and Metabolic Pathway Similarity) uses the ChEBI (Chemical Entities of Biological Interest) [7] ontology to calculate semantic similarity between chemical compounds and also between pathways from the Kyoto Encyclopedia of Genes and Genomes (KEGG) [8] by comparing the sets of ChEBI terms associated with them. The integration of ChEBI-based semantic similarity has been shown to improve existing chemical compound classification systems [9]. CMPSim is also able to find the most meaningful chemical compound classes in a set of pathways, highlighting their common properties.

GRYFUN (GRaph analyZer of FUNctional annotation) supports the visualization of functional profiles of protein sets. These profiles are structured as subgraphs of GO, showing the terms annotated to the protein set and allowing a global view of its functional broadness and specificity. They also provide detailed statistics and relevant metrics by integrating data from GO and UniProt, and support the selection of protein subsets sharing a specific profile. GRYFUN is currently restricted to a dataset of carbohydrate-active enzymes.

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